Title: Protein Binding and Interaction Analysis of Human Pathogen Targets

Principal Investigator: T. Andrew Binkowski, *Argonne National Laboratory (ANL)*

Co-Investigator: Wei Jiang (*ANL*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 22,800,000 processor hours

Research Summary:
Proteins play a fundamental role in cells and living organisms, including serving as nanoparticle sized bio-machinery that enables the chemical reactions necessary for life. Ligands are biomolecules that bind to proteins and are either acted upon by the protein or are used to control the protein function. Because the protein-ligand interaction is crucial to all living organisms, understanding and controlling these interactions is important across many scientific disciplines (i.e. biology, chemistry, physics) and in many different arenas (i.e. academic, government, industry). However, despite continued advancement in experimental biology techniques, the inherent limitations of time and expense severely limit our ability to fully characterize and study protein-ligand interactions. It is becoming clear that biomolecular simulation is becoming a necessary method for advancing our knowledge of protein-ligand interactions. Simultaneous with the growing need for simulations, advances in high-performance computation are allowing computationally expensive algorithms to be implemented, driving breakthroughs in molecular modeling and simulation. In this project, we propose to leverage the vast computing resources available to operate a workflow that merges state-of-the-art methods in molecular modeling and simulation into a single computational pipeline. The pipeline will be applied to study important proteins in infectious disease and human health. The outcomes of this project will include insights into protein-ligand interactions and demonstrate a more broadly applicable approach for leveraging high performance computing resources to investigate ligand-protein interactions.

Title: Massive Monte Carlo Simulations For the Analysis of Planck Satellite Data

Principal Investigator: Julian Borrill, *Lawrence Berkeley National Laboratory/UC Berkeley*

ALCC allocation: Processor Hours
Site: Lawrence Berkeley National Laboratory
Allocation: 5,000,000 processor hours

Research Summary:
The Planck satellite is part of a mission to measure the faint echo of the Big Bang. In 2014/15 the Planck collaboration will release its final results, providing powerful constraints on the fundamental parameters of cosmology and high-energy physics and setting the stage for the next generation of Dark Energy experiments. Obtaining precise Planck results will require massive Monte Carlo simulation sets that can only be generated on the largest supercomputers. This proposal will support the generation of cosmic-microwave background Monte Carlo set and help yield insights into Dark Energy.

Title: Structure and Dynamics of Nuclear Systems within Time-Dependent Density Functional Theory Approach

Principal Investigator: Aurel Bulgac, *University of Washington*

Co-Investigators: K. J. Roche (*PNNL and U. Washington*), I. Stetcu (*LANL*), P. Magierski (*Warsaw U. Technology and U. Washington*), J. W. Holt (*U. Washington),* C. Bertulani (*Texas A&M*), M. M. Forbes (*U. Washington and Washington SU*), Y. Yu (*Chinese Academy of Sciences*), G. Wlazlowski (*Warsaw U. Technology and U. Washington)*

ALCC allocation: Processor Hours

Site: Oak Ridge National Laboratory

Allocation: 25,000,000 processor hours

Research Summary:

The structure and dynamics of nuclear systems is critical to the origins of the elements, the structure of stars, and applications in energy and defense. To further our understanding of nuclear systems, it is important that theoretical models and simulations be developed in conjunction with high performance computing resources. Over the last several years we developed codes (superfluid and time-dependent extensions of the Density Functional Theory (DFT) approach) for studying nuclear systems on leadership computing resources. This project will use these state of the art codes to study a range of low energy nuclear reactions, in particular induced nuclear fission, where nuclear superfluidity is an essential element. The outcomes of this project will provide more detailed theoretical understanding of nuclear systems that supports the wide range of application areas depending on this knowledge.

Title: Ab Initio Quantum Liquid Water and Aqueous Ionic Solutions

Principal Investigator: Robert A. DiStasio Jr., *Princeton*

Co-Investigators: Roberto Car (*Princeton*), Biswajit Santra (*Princeton*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 250,000,000 processor hours

Research Summary:

A highly accurate and detailed understanding of the microscopic structure of liquid water is of great importance to a number of fields, including energy storage, biochemistry, and the environmental sciences. At present, there is no experimental methodology available to directly obtain the real-space microscopic structure of liquid water. Computer-based simulations can furnish such structural information in a relatively straightforward manner; however, the state of the art computational approach for microscopic molecular modeling (*ab initio* molecular dynamics (AIMD)) has severe limitations when applied to liquid water. This project will address key challenges of AIMD liquid water simulations and apply the developments in a series of benchmark simulations on liquid water and ionic solutions relevant to aqueous ion batteries. These simulations will enable a highly accurate understanding of the microscopic structure of liquid water and yield insights on several important issues pertinent to the understanding and rational design of aqueous ion batteries. The results will be stored in a publicly available structural database to serve as an invaluable resource for further simulation developments, exploration by the wide range of scientific stakeholders (e.g., biologists, electrochemists, environmental scientists), and the benefit of the broader scientific community.

Title: LES of SFR Assembly Inlets

Principal Investigators: Paul Fischer, *Argonne National Laboratory (ANL),* James Tallman *(General Electric)*

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 60,000,000 processor hours

Research Summary:
Nuclear reactors provide a safe, carbon free source of energy and are a key component of domestic clean energy production. Improving nuclear reactor design is therefore important for increasing the utility and energy efficiency of this important energy source. In current reactor designs, excess heat produced in the nuclear reactor is cooled by water. Although the water cooling system controls the reaction process, efficiency is lost as water slows the speed of the neutrons (an important particle to the nuclear reaction process). The lost efficiency translates into greater nuclear waste products and less energy efficient reactors. A sodium cooled fast reactor (SFR) is a promising alternative to a water cooled reactor. However, challenges in SFR safety and design have hindered their implementation. An important safety aspect of the SFR design is that the reactor core be free of moving parts and the coolant flow driven by buoyancy induced by the heat of the fuel rods. Control of the coolant flow rate and, hence, cooling is determined by controlling pressure drops in the flow path for each of the several hundred assemblies in the reactor. Knowing these pressure drops as a function of flow rate is crucial to the reactor design process.This project supports simulations to examine two successive components in the flow path, namely, the assembly entrance port and the orificing plate stack, components crucial to the overall design process. The outcome of this work will be a greater understanding of controlling cooling in SFR and an important step towards building better, safer, and more energy efficient nuclear reactors.

Title: Predictive Full-Scale Simulations of Fast Ignition of Fusion Targets

Principal Investigator: Frederico Fiuza, *Lawrence Livermore National Laboratory (LLNL)*

Co-Investigators: Andreas Kemp (*LLNL*), Anthony Link (*LLNL*), Bruce Cohen (*LLNL*), Warren Mori (*UCLA*), Luis Silva (*IST, Portugal*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 19,500,000 processor hours

Research Summary:
Fusion energy is regarded as a possible long term energy solution for humanity, capable of providing the energy resources to drive economic growth and social development. Fast ignition is one of the most promising and scientifically exciting schemes to improve the viability of inertial fusion energy as a practical energy source. In fast ignition, the heating of a compressed core is provided by injecting high energy (tens of kilojoules of total energy) electrons into the fusion target. The electrons are generated by a short pulse laser. Up to now, short pulse laser experiments have been limited to energies still far from ideal conditions for ignition. Additionally, the simulations, which are extremely complex, have been limited to reduced spatial and temporal scales and to simplified models. This project aims to perform the first full scale three dimensional simulations of fast ignition, with realistic target properties (e.g. density, temperature, dimensions). The simulations will capture the multi scale physics associated with the laser plasma interaction, fast electron transport and energy deposition in a self consistent manner. This proposal will take advantage of a suite of massively parallel, highly optimized codes, with the goal of identifying a path to demonstrate fast ignition as a viable scheme for inertial fusion energy.

Title: First Principles Investigations of Adsorbate-Metal Interactions: Quantum Monte Carlo and Ab Initio Molecular Dynamics Simulations

Principal Investigator: Jeffrey Greeley, *Purdue University*

Co-Investigator: Jeongnim Kim (*ORNL*)

ALCC allocation: Processor Hours

Site: Argonne National Laboratory
Allocation: 50,000,000 processor hours

Site: Oak Ridge National Laboratory
Allocation: 25,000,000 processor hours

Research Summary:
The chemistry and physics of water near metal surfaces is central to a host of critical technological applications, ranging from metal corrosion to fuel cell electrocatalysis. Experimental studies of water-metal interactions, while providing very useful information about single molecule or monolayer water adsorption on metals, are restricted to low temperatures and provide no direct insights into how bulk water reorganizes itself near metal surfaces. Computational studies, on the other hand, are suited to understanding the molecular-level details of water adsorption on surfaces. This project will advance the theoretical accuracy of current state-of-the art simulation approaches . New Quantum Monte Carlo and ab-initio molecular dynamics-based approaches will be used to explore novel aspects of the interaction of molecules that are central to electrocatalytic reactions and fuel cell science, including water, carbon monoxide, and nitrogen-containing compounds, with transition metal surfaces. These results will improve theoretical understanding of water metal interactions and provide improved technology for prediction and development in the various technological applications related to water-metal interactions.

Title: Unravelling the Coupling of Radio Frequency Power to Fusion Plasmas

Principal Investigator: David Green, *Oak Ridge National Laboratory* (*ORNL*)

Co-Investigators: Erwin F. Jager (*ORNL*), Lee A Berry (*ORNL*), Ed D'Azevedo (*ORNL*), Paul T. Bonoli (*MIT*), John C. Wright (*MIT*), David Smithe (*Tech-X*), Cynthia K. Phillips (*PPPL*), Erntes J. Valeo (*Princeton Plasma Physics Laboratory*), Dan D'Ippolito (*Lodestar*), Jim R. Myra (*Lodestar*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 50,000,000 processor hours

Research Summary:
The International Thermonuclear Experimental Reactor (ITER) is a multinational project to test magnetically confined nuclear fusion as a commercial, base-load source of electrical power. Success in ITER would be invaluable for finding a clean renewable source of energy for the world. This success is defined as achieving plasma ignition and fusion power production of greater than 10 times the power consumed (Q≥10), and will depend on efficient external plasma heating (a total of 50 MW). The external heating systems presently slated for ITER are neutral beam injection and radiofrequency (RF) heating in both the electron cyclotron and ion cyclotron frequency ranges. Of these heating technologies, the ion cyclotron RF heating (ICH) is the most cost effective. However, ICH suffers from parasitic power losses that are not well understood. This project will support 3D simulations that have the required resolution and physics to provide an understanding of the parasitic losses. This understanding may significantly help improve external heating efficiency, and further the efforts to the ITER goal of Q≥10. The outcome of this project will be an advancement of controlled fusion science and its practical application as a source of clean energy.

Title: Controlling Nanoparticle Assembly to Engineer New Materials

Principal Investigator: Gary S. Grest, *Sandia National Laboratories (SNL)*

Co-Investigators: Sanat K. Kumar (*Columbia University*), Dvora Perahia (*Clemson University*), Steve J. Plimpton (*SNL*), Mark O. Robbins (*Johns Hopkins University*), Mark J. Stevens (*SNL*)

ALCC allocation: Processor Hours
Site: Lawrence Berkeley National Laboratory
Allocation: 40,000,000 processor hours

Research Summary:
A new realm of materials and devices will result from our ability to control the integration of nanoparticles (NPs) into these materials and devices. Controlled integration of NPs will allow the enhanced mechanical and optical characteristics in the nano dimension to be transposed into large scale devices. However, the need to integrate the particles into devices without losing their unique properties remains a challenge. Using leadership computing resources, we have already gained significant insight on the effects of the strength, length scale and directionality of the inter-particle interactions. This project will further probe the forces that control the symmetry of NP assemblies and correlate them with the properties of the systems. The outcome of this project will be an important step towards overcoming the major barriers to integrating NPs into a range of advanced devices, controllably dispersing and organizing them within durable matrices while retaining their unique properties.

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Title: Design of High-Efficiency Solar Thermal Fuels via First Principles Computations

Principal Investigator: Jeffrey Grossman, *Massachusetts Institute of Technology*

ALCC allocation: Processor Hours
Site: Lawrence Berkeley National Laboratory
Allocation: 30,000,000 processor hours

Research Summary:
Harnessing sources of clean and renewable energy is one of the most important global topics of this century. Full utilization of the largest potential source of renewable energy — the sun — requires advanced technologies for converting light into forms of energy that can be stored for convenient transport and on-demand use. Recently, an energy storage approach using solar thermal fuels (STFs) has garnered attention. Solar thermal fuels (STFs) store energy from the sun in the chemical bonds of molecules and are a promising approach to clean energy storage and conversion. However, adaptation of STFs as a viable, low-cost, large-scale means of energy storage and conversion will require the discovery of new materials that can efficiently make use of the solar spectrum. This project will run simulations to investigate the optical and thermodynamic properties of STFs for an improved knowledge of the photochemistry and photophysics of the molecular materials under study. The approach has the potential to lead to a deeper understanding of the fundamental relationships between chemical structure and energy storage potential in the large class of photoactive molecular materials for STFs. The final goal is to enable systematic design of STFs with optimized quantum yield, photostationary state composition, and sunlight absorption in addition to favorable thermal and energetic properties.

Title: Titan-Enabled Supersonic CCS Compressor and Engine Technology Development: Intelligently-Driven Optimization, Time-Varying Boundary Layer Flow Control, and GPU-Accelerated Convergence Augmentation

Principal Investigator: Allan Grosvenor, *Ramgen*

Co-Investigators: Norbert Podhorszki (*ORNL*), Charles Hirsch (*Numeca*)

ALCC allocation: Processor Hours

Site: Oak Ridge National Laboratory

Allocation: 20,000,000 processor hours

Research Summary:

Power plants burning fossil fuels account for more than 40 percent of the world's energy-related CO2 emissions and will continue to dominate the supply of electricity until the middle of the century. There is therefore an urgent need for cost-effective methods to capture and store their carbon emissions. The principal barrier to widespread application of carbon capture and sequestration (CCS) is its cost. Once the CO2 is captured, compressing it to the required 100 atmospheres represents approximately 33 percent of the total cost of CCS. This project supports the development of shock wave compression technology (turbomachinery operating in the supersonic relative flow regime) to reduce the cost of Carbon Dioxide compression for CCS. Introducing shock wave compression technology into a carbon capture process may enable excess heat energy produced by the CCS process to be 'put to work' in the electric generation process. Harvesting the excess heat energy in this manner would reduce the net energy and financial costs of CCS. The outcome of this project will be a better understanding of a promising technology for cost effective CCS and a step towards cleaner electric energy production.

Title: Coupled Hydro-Geophysical Inversion of River Water Intrusion and Biogeochemical Transport Modeling at the Hanford 300 Area

Principal Investigator: Glen Hammond, *Pacific Northwest National Laboratory (PNNL)*

ALCC allocation: Processor Hours
Site: Lawrence Berkeley National Laboratory
Allocation: 16,000,000 processor hours

Research Summary:
The Hanford 300 Area was a United States site used for plutonium and weapons production. These activities left solid and liquid wastes that pose a risk to the local environment. Modeling system-scale groundwater-river water mixing and exchange at the Hanford 300 Area is therefore important to evaluate the extent of the environmental risks caused by the waste. The mixing process greatly impacts water chemistry and subsequently soil microbial life at the site as the river water chemistry can differ significantly from that of the groundwater. The purpose of this research is to determine environmentally important hydrologic parameters through computer simulation incorporating experimental data from groundwater monitoring and geophysical investigations. The parameters will create an optimized hydrologic model that will be employed to simulate the fate and transport of microbial populations at the site. The project will enable prediction of biogeochemical transport within the Hanford 300 Area, investigation into the long-term microbial ecology within the site, and assessment of indirect climatic impacts to biogeochemical cycles within the domain. The outcome will be an improved understanding of the local biogeochemical cycle and the migration of contaminants at the site.

Title: First-principle Investigation of Oxygen Defects in Metal/Oxide/Metal Heterostructures: Structure, Energetics, and Transport in the Quantum Regime

Principal Investigator: Olle Heinonen, *Argonne National Laboratory (ANL)*

Co-Investigator: Ivan Rungger (*Trinity College, Dublin Ireland*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 50,000,000 processor hours

Research Summary:
Oxides and oxide heterostructures are important materials found in micro-electronics including ferroelectric capacitors and memories, as well as in electroceramics. Oxide heterostructures – metal/oxide/metal sandwiches - are key components to 'resistive switches' that are currently intensively researched for applications in non-volatile memory storage. Oxygen defects in these oxide and oxide heterostructures profoundly affect the behavior of these materials and their implementation as resistive switches. The structure, energies, and arrangement of oxygen defects in the presence of metal electrodes must be well understood in order to arrive at a microscopic understanding of resistive switching, yet there is surprisingly little theory and modeling work in the literature on oxygen defects in resistive-switching structures. In addition to calculating energetics and local structures, it is desirable to be able to directly calculate the transport properties, such as electrical conductivity, of metal/oxide/metal structures. The theoretical modeling structures published to date involve a relatively small number of atoms and are limited to oxygen defects in the oxide matrix and do not include interfaces with a metal electrode, nor do they include transport calculations. The objective of the proposed research is to elucidate the fundamental mechanism of resistive switching in metal/oxide/metal heterostructures. Outcomes of this project will advance molecular understanding of these important materials with applications in ferroelectrics, catalysis, multiferroics, and other complex oxides for novel functionalities.

Title: MockBOSS: Calibrating Boss Dark Energy Science with HACC

Principal Investigator: Katrin Heitmann, *Argonne National Laboratory (ANL)*

Co-Investigators: Daniel Eisenstein (*Harvard*), Nikhil Padmanabhan (*Yale*), Hal Finkel (*ANL*), Tomomi Sunayama (*Yale*), Salman Habib (*ANL*), Martin White (*UC Berkeley*), Adrian Pope (*ANL*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 47,000,000 processor hours

Research Summary:
Cosmic acceleration describes the observation that the Universe is expanding at an increasing rate. Understanding the underlying cause of cosmic acceleration is one of the great problems in physics and is being observationally probed by large cosmological surveys. In particular, spectroscopic galaxy surveys like the Baryon Oscillation Spectroscopic Survey (BOSS, ongoing) and the future Mid Scale-Dark Energy Spectroscopic Instrument (MS-DESI) are characterized by high precision and exquisite levels of control over systematic errors. Large-scale simulations tuned to the requirements of these surveys are essential for extracting the science contained within the observations. Simulations also establish the robustness of the results obtained and serve as a defense mechanism against systematic uncertainties. This project will carry out a large set of N-body simulations optimally designed in their size, resolution, and throughput, to further BOSS science goals. The simulation results will be an unprecedented resource for BOSS and will lead to major advances in three directions (i) control of systematic effects in baryon acoustic oscillation measurements, (ii) enabling new approaches to covariance matrices, and (iii) calibrating redshift (distant) space distortions as a dark energy and modified gravity probe for BOSS. The outcome of this research will be to enhance interpretation of BOSS survey data and further theoretical understanding of cosmic acceleration.

Title: Exploring the Chemical Landscape for Base Excision DNA Repair

Principal Investigator: Ivanov Ivaylo, *Georgia State University*

ALCC allocation: Processor Hours
Site: Lawrence Berkeley National Laboratory
Allocation: 3,000,000 processor hours

Research Summary:
Despite its remarkable stability, DNA is subject to a variety of reactions. Left unchecked, these processes could impair the transmission of vital genetic information and, thus, threaten the integrity of the genome. DNA is composed of a series of bases and one of the most essential components to maintaining correct DNA is the identification and repair of damaged bases. The process of fixing incorrect bases is called base excision repair (BER) and is accomplished by enzymes, BER enzymes. This project supports efforts to understand the detailed mechanisms of BER. Two general themes are explored: (i) the interaction between the BER enzymes and DNA, e.g. how does the enzyme identify, excise and repair only the damaged base? And (ii) what are the mechanistic steps for the excision and repair process? We will apply state-of-the-art *ab initio* molecular dynamics (AIMD) methods to shed light on these important issues. This proposal is directed toward development and application of computational methods to address topical issues in the field of DNA repair. The projected outcomes will substantially impact our knowledge of the biochemical pathways controlling genetic integrity with relevance to the mission of DOE.

Title: Study of the Internal Dynamics of ITER

Principal Investigator: Stephen C. Jardin, *Princeton Plasma Physics Laboratory (PPPL)*

Co-Investigators: Nate Ferraro (*General Atomics*), Mark Shephard (*RPI*)

ALCC allocation: Processor Hours
Site: Lawrence Berkeley National Laboratory
Allocation: 20,000,000 processor hours

Research Summary:
The International Thermonuclear Reactor Experimental Reactor (ITER), now being constructed in Cadarache, France, is a monumental step towards the realization of fusion power. Success in this endeavor will be a turning point in the quest for a sustainable, carbon free, and safe source of energy for the planet. To facilitate the realization of ITER success, this project will use a state-of-the-art extended magnetohydrodynamics code to model the internal global dynamics of the high-temperature ionized gas (plasma) within ITER. The project goals are to accurately model and predict the onset of instabilities and reconnection events that will occur in ITER (and other magnetic fusion devices) due to slowly changing boundary conditions and the slow evolution of pressure and current density profiles due to applied and internal heating and transport processes. The new understanding provided by the simulations will provide guidance for the different modes of operation and optimization and control strategies to be used for ITER. These outcomes will support the ITER mission of demonstrating the practicality of clean, renewable, fusion energy.

Title: Projections of Ice Sheet Evolution

Principal Investigator: Philip Jones, *Los Alamos National Laboratory (LANL)*

Co-Investigators: William Lipscomb (*LANL*), Matthew Maltrud (*LANL*),Stephen Price (*LANL*), Doug Ranken (*LANL*), Esmond Ng (*LBNL*), Daniel Martin (*LBNL*), Kate Evans (*ORNL*), Matthew Norman (*ORNL*), Pat Worley (*ORNL*), Andrew Salinger (*SNL*), Michael Eldred (*SNL*), Irina Kalishnikova (*SNL*), Mauro Perego (*SNL*), Bill Sacks (*NCAR*), Charles Jackson (*U. Texas*), Lili Ju(*U. South Carolina*)

ALCC allocation: Processor Hours

Site: Lawrence Berkeley National Laboratory
Allocation: 5,000,000 processor hours

Site: Oak Ridge National Laboratory
Allocation: 2,600,000 processor hours

Research Summary:
Sea-level rise is potentially one of the most significant consequences of future climate change, posing risks to coastal populations, infrastructure end ecosystems. Mass loss from the large ice sheets in Greenland and Antarctica is accelerating and will become the dominant contributor to future sea level rise due to climate change. This project supplies computing resources for developing new ice sheet and climate model components to improve our capability to project future ice sheet and sea level changes. Testing is underway for new multi-scale dynamical formulations to better represent ice sheet processes along ice streams, outlet glaciers and at the ice sheet margins. Validation frameworks are also being created for exploration and performance evaluation of ice sheet models. The outcomes will support a better understanding of ocean-ice sheet interactions around the Antarctic continent and increase predictive capabilities of sea-level rise.

Title: Gyrokinetic Simulation of Energetic Particle Turbulence and Transport

Principal Investigator: Zhihong Lin, *UC Irvine*

Co-Investigators: Ihor Holod (*UC Irvine*), Ronald Waltz (*General Atomics*),Donald Spong (*ORNL*), Peng Wang (*NVIDIA*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 50,000,000 processor hours

Research Summary:
The International Thermonuclear Experimental Reactor (ITER) is a multinational collaboration to advance developments of fusion as a source of clean and renewable energy. One challenge in ITER burning plasma experiment is that the fusion reactions produce energetic particles, which constitute a significant fraction of the local plasma energy density. Collectively, these energetic particles can excite electromagnetic instabilities which could adversely affect the overall performance and even damage the device of ITER. The most prominent type of instability is called the shear Alfvén wave (SAW) that could drive large transport of energetic particles. This project supports first-principles global (macro scale) simulations to study new physics including Alfvén wave turbulence and the transport of energetic particles with kinetic physics on micro and meso scales. The outcomes will help accurately predict confinement properties of energetic particles in burning plasmas and support the goals of engineering a stable fusion reactor.

Title: Simulating Cosmological Lyman-alpha Forest

Principal Investigator: Zarija Lukic, *Lawrenece Berkeley National Laboratory (LBNL)*

Co-Investigators: Ann Almgren (*LBNL*), Peter Nugent (*LBNL*)

ALCC allocation: Processor Hours
Site: Lawrence Berkeley National Laboratory
Allocation: 24,000,000 processor hours

Research Summary:
Dark energy and dark matter together account for 95% of the mass-energy of the Universe, yet both remain mysterious and little well understood. The observations from ongoing Baryon Oscillation Spectroscopic Survey (BOSS) and a next-generation Mid-Scale Dark Energy Spectroscopic Instrument (MS-DESI) survey will serve as a gold mine for understanding the evolution of the universe and the nature of these two mysterious components. However, interpreting such observations is impossible without theory, modeling, and simulation efforts. On the theoretical side, the main roadblock to interpreting observations is a lack of precise predictions for a subtle signal, easily masked by inadequately understood astrophysical systematic errors. The only known way to accurately model the complex non-linear evolution of matter, and to do it at the level of accuracy required by the sky surveys, is through large-scale cosmological simulations. This project will study clustering of matter in the high redshift (distant) universe. In particular, we will focus on cosmological simulations of the Lyman-alpha forest, and its role as a measurement tool for the power spectrum of the matter fluctuations. The outcome of this project is to further establish a computation-based discovery capability for critical cosmological probes and better enable observatories to provide crucial information related to dark energy and dark matter.

Title: High-Fidelity Simulations of Transition and Turbulent Separation in Turbomachinery

Principal Investigator: Gorazd Medic, *United Technologies Research Center*

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 10,000,000 processor hours

Research Summary:
Improvements in turbomachinery components are of key importance to the development of next generation fuel efficient commercial jet engines. Turbomachinery flows contain several features that have over the years proven to be an important challenge for turbulence models widely used in industry. Examples of these features include strong rotational and curvature effects, as well as laminar-to-turbulent transition. This project will focus on high-fidelity modeling for realistic three-dimensional turbomachinery configurations and the outcome of this project will lead to improvements in the understanding and modeling of turbomachinery flows. Our ability to better understand the flow physics will help lead future design improvements and will be critical to improved energy efficiency of turbomachinery components.

Title: Petascale Thermal Hydraulic Simulations in Support of CESAR

Principal Investigator: Elia Merzari, *Argonne National Laboratory*

Co-Investigators: Paul Fischer (*ANL*), Justin Walker (*ANL*),Andrew Siegel (*ANL*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 80,000,000 processor hours

Research Summary:
Safer nuclear energy power promises to become a reliable, carbon-free resource capable of meeting our nation's and the world's energy needs. Numerical simulation has been an intrinsic part of nuclear engineering research, design, and licensing of existing and proposed conventional nuclear power plants. Nuclear modeling and simulation tools available today, however, are mostly low dimensional, empirically based, valid for conditions close to the original experiments, and in many cases incremental improvements on decades-old legacy codes. The development, deployment, verification, and validation of higher-fidelity computational capabilities for analyzing, modeling, simulating, and predicting complex thermo-fluid phenomena will help advance nuclear power capabilities by resolving technical, cost, and safety issues. The Center for Exascale Simulation for Advanced Reactors (CESAR), one of the three codesign centers funded by DOE, aims to address these challenges by developing a coupled, next generation nuclear reactor core simulation tool capable of efficient execution on exascale computing platforms. This project supports the mission of CESAR with large petascale level simulations needed to address the limitations of current methods and address the potential scaling to larger machines. The resulting improved state-of-the art simulation code will aid advancements in nuclear engineering and nuclear energy.

Title: Multiscale Modeling of Dynamic Arctic Landscapes in a Changing Climate

Principal Investigator: Richard Mills, *Oak Ridge National Laboratory (ORNL)*

Co-Investigators: Gautam Bisht (*LBNL*), Glen Hammond (*PNNL*),Forrest Hoffman (*ORNL*), Satish Karra (*LANL*), Jitendra Kumar (*ORNL*), Peter Lichtner (*OFM Research*), Scott Painter (*LANL*), William Riley (*LBNL*), Peter Thornton (*ORNL*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 30,000,000 processor hours

Research Summary:
Reliable projections of climate are vital for science and policy decisions relating to climate change mitigation and adaptation. Advances in our understanding have enabled the development of increasingly sophisticated Earth System Models (ESMs), but model predictions are still hampered by uncertainties in the representation of some key processes. One key source of uncertainty is modeling Arctic carbon release. Arctic and sub-Arctic soils have been a net sink of carbon for thousands of years and currently contain approximately 1700 billion metric tons of frozen organic carbon, approximately 200 times the annual anthropogenic release. This vast amount of frozen carbon is vulnerable to release to the atmosphere in the form of carbon dioxide and methane as Arctic temperatures warm. The timing and rate of Arctic carbon release to the atmosphere is therefore a critical uncertainty in understanding the trajectory of the Earth's climate system. This project will increase confidence in ESM predictions by improving the representation of biogeochemical processes in Arctic tundra ecosystems. Using a set of nested model sub-domains, the project will conduct a series of simulations of permafrost-affected landscapes within an 'upscaling/downscaling' framework. By *upscaling* the results from small-scale models we hope to optimally inform process representations at the global climate model scale; by *downscaling* results from the global climate model scale, we hope to provide appropriate large-scale context for simulations conducted at smaller scales. The ultimate goal is to improve the representation of Arctic eco-climatological processes at the scale of a high-resolution Earth System Model and advance the reliability of climate change projections.

Title: Wall Modeling and Primary Atomization for Predictive Large-Eddy Simulation of Airframes, Jet Engines and Jet Noise

Principal Investigator: Parviz Moin, *Stanford University*

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 150,000,000 processor hours

Research Summary:
Predictive large-eddy simulation (LES) of realistic high Reynolds number (high speed) flows is critical to engineering analysis and design of aerospace systems including, airplanes, jet engines, fuel injectors and turbines. This project will address two key challenges in large-eddy simulation (LES) of high speed flows: wall modeling of turbulent boundary layers and primary atomization of liquid jets. Four high-risk, high-payoff simulations will be developed that leverage the 'CharLes' codebase to significantly advance the state-of-the-art in LES technology by solution of (i) a full airframe wing/body high-lift system, (ii) a three-dimensional, transiently stalled diffuser, (iii) complex geometry supersonic jet nozzle with turbulent inflow and (iv) primary breakup of turbulent liquid jets in crossflow. The anticipated results of this research are (i) the first ever LES of the benchmark NASA Trap Wing with validation against both wind tunnel tests and data from the 2010 AIAA High Lift Prediction Workshop, (ii) LES of a stalled diffuser using a novel and more accurate modeling approach, (iii) a new understanding of how to model the flow inside complex geometry nozzles and its effects on the nozzle-exit boundary layer, the jet exhaust and ultimately the aeroacoustic field, and (iv) verification and validation of a new two-phase flow predictive algorithm. The results will improve the realism of simulations for high speed flows and further enable next-generation engineering of energy efficient and environmentally sound advanced technology devices.

Title: Does A Turbulent Duct Flow Ever Become Two-Dimensional

Principal Investigator: Hassan Nagib, *Illinois Institute of Technology/KTH Mechanics, Sweden*

Co-Investigators: R. Vinuesa (*Illinois Institute of Technology*), P. Schlatter (*KTH Mechanics, Sweden*),A. Obabko (*Argonne National Laboratory*), P. F. Fischer (*Argonne National Laboratory*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 11,000,000 processor hours

Research Summary:
The flow of fluids in ducts with rectangular cross-section is frequently encountered in a variety of environmental, technical and even biological applications. Typical examples of duct flows can be found in urban drainage systems, ventilation systems and combustion engines. Of particular importance in flows delimited by solid walls is the near-wall region in which a large fraction of the drag stems from velocity fluctuations in a thin boundary layer adjacent to surfaces. This project supports numerical simulations aimed at assessing the three-dimensional effects present in turbulent duct flows, as well as their dependence on the duct geometry. This project has two main goals: first, this study will provide a deeper fundamental understanding of wall-bounded turbulence, and of the mechanisms responsible for the convergence from low to high aspect ratio behavior in the duct. Second, the data collected in this project will help to develop more accurate turbulence models, since the currently available industrial codes still fail to accurately predict three-dimensional flows with secondary motions. The results are expected to have profound impact on our understanding of comparisons between modern and classical canonical experiments, and the largest volume of direct numerical simulation data in the literature.

Title: Large-Scale Computation for Discovery and Design of Excited State Phenomena in Next-Generation Energy Conversion Materials

Principal Investigator: Jeffrey B. Neaton, *Lawrenece Berkeley National Laboratory (LBNL)*

Co-Investigators: Andrew Canning (*LBNL*), James R. Chelkowsky (*UT Austin*), Jack Deslippe (*LBNL*), Steven G. Louie (*UC Berkeley/ LBNL*), Yousef Saad (*U. of Minn),* Chao Yang (*LBNL*)

ALCC allocation: Processor Hours

Site: Argonne National Laboratory
Allocation: 23,000,000 processor hours

Site: Lawrence Berkeley National Laboratory
Allocation: 18,000,000 processor hours

Research Summary:
New materials and phenomena are needed to realize low-cost, efficient, and sustainable conversion of sunlight into usable and clean forms of energy. Organic assemblies and transition-metal oxides comprise two promising classes of materials in this respect, and are of considerable interest for many next-generation solar energy applications, including photovoltaics and photocatalysis. The ability to tune these materials systems for solar energy conversion hinges on an understanding of the connection of their ground-state structure and atomic-scale geometry o their so-called “excited-state” properties, such as optical absorption, charge transport, and charge separation. This program will address precisely this challenge, and lead to new understanding and predictive capabilities for structural, optical, and related excited state properties of a broad array of photoactive organic molecules and solids, transition-metal oxides, and their interfaces with an eye toward next-generation solar energy conversion. In tandem with laying the groundwork for a ‘materials genome’-like database for such systems, the project will address important outstanding questions related to the performance of state-of-the-art algorithms and computational methods for describing ground- and electronic excited-state properties of complex organic- and oxide-based materials. The result will be improved abilities to predict electronic excited-state properties in complex materials, as well as new principles relating these phenomena to underlying atomic structure and chemical composition, both of which are central to the identification of next-generation energy conversion materials for harnessing sunlight into clean, renewable energy.

Title: U.S. Russia Collaboration on Cross-Verification and Validation in Thermal Hydraulics: Nek5000, Cfoam-CABARET, and Conv3D, Simulations of MATiS and MAX Experiments

Principal Investigator: Aleksandr Obabko, *Argonne National Laboratory (ANL)*

Co-Investigators: Paul Fischer (*ANL*), Justin Walker (*ANL*),Vladimir V. Chudanov (*IBRAE, Russia*), Valeriy A. Pervichko (*IBRAE, Russia*), Anton A. Kanaev (*IBRAE, Russia*), Vasily M. Goloviznin (*IBRAE, Russia*), Mikhail A. Zaytsev (*IBRAE, Russia*), Sergey Karabasov (*QMUL, UK*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 44,000,000 processor hours

Research Summary:
Safer nuclear energy promises a reliable, carbon-free power resource capable of meeting the nation's and the world's energy needs. One of the critical safety parameters in a nuclear power plant is the peak material temperature. Prediction of the peak temperature involves accurate computation of thermal hydraulics with large-eddy simulations (LES). This project focuses on validation and cross-verification of three thermal hydraulics LES codes with benchmark experiment MATiS and data from ANL's MAX facility (a fluid dynamics test facility). The outcomes of this project will improve state of the art computational simulation capabilities and will advance an international engagement in support of the safe, secure, and peaceful use of nuclear energy.

Title: Accelerating Design of Complex Fuel Injectors Through Petascale Computing

Principal Investigator: Madhusudan Pai, *GE Global Research*

Co-Investigators: Olivier Desjardins (*Cornell University*)

ALCC allocation: Processor Hours

Site: Oak Ridge National Laboratory
Allocation: 46,000,000 processor hours

Research Summary:
Automobile and aviation engine manufacturers are actively engineering more energy efficient and environmentally friendly engines. Engines that rely on liquid fuel combustion have evolved over time with more complex subcomponents of which the fuel injection system is perhaps the most critical and challenging to design. Fuel injectors, therefore, are the focus of a particularly intensive design optimization cycle. The principal challenge in designing today's complex fuel injectors is the need to identify and understand the impact of small changes in fuel injector geometry that lead to improvements in engine performance. To address this challenge, it is vital that we first obtain a detailed physical understanding of unsteady fuel spray breakup from complex fuel injector geometries. Experiments alone are limited in their ability to probe regions inside the injector where spray breakup is initiated. This project will perform simulations to answer the following questions: How do small changes to complex fuel injector geometry modify spray behavior? What are the physical mechanisms that underlie this change in injector behavior? What is the potential for HPC to accelerate design of complex fuel injectors through systematic design sensitivity studies performed on massively parallel supercomputers, thereby reducing development cycle times? The outcome of this work will serve as a stepping stone towards the development of clean burning liquid-fueled combustion engines using HPC.

Title: Simulation the Structure and Dynamics of Protein Kinase A

Principal Investigator: Loukas Petridis, *Oak Ridge National Laboratory (ORNL)*

ALCC allocation: Processor Hours
Site: Lawrence Berkeley National Laboratory
Allocation: 4,000,000 processor hours

Research Summary:
Protein Kinase A (PKA) helps regulate the function of proteins involved in a variety of cellular processes. Protein Kinase A functions by phosphorylating (adding phosphate groups) target proteins in response to an increase in cyclic adenosine monophaste (cAMP) which binds to PKA and triggers activity. The phosphorylation of the protein then impacts the protein function allowing cAMP and PKA to regulate the protein. This project supports a series of simulations to understand the structure and dynamics of this complex of proteins. The project seeks to understand how events related to the binding of cAMP to PKA translate into the changes that enables the function of PKA. The results of the simulations will be used to interpret the results of neutron scattering experiments performed on the PKA subunits and their complexes. This project will thus explore new frontiers in biology. Furthermore the demonstration of how high-performance computing can be integrated with neutron scattering experiments in biological research will broaden the community of researcher's that use leadership computing resources.

Title: The Role of Aerosols and Multi-scale Water Cycle Processes in Climage Change: Sensitivity to Aerosol Emissions and Modeling Frameworks

Principal Investigator: Philip Rasch, *Pacific Northwest National Laboratory (PNNL)*

Co-Investigators: L. Ruby Leung (*PNNL*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 36,000,000 processor hours

Research Summary:
Climate simulations are invaluable for developing theoretical understanding of climate and for predicting future change and impacts. The value of the predictive capability of climate models may be significantly attenuated by various sources of uncertainty. Among the sources of uncertainties, the impacts of model resolution may be most wide ranging because it exposes a key limitation of how physical processes are represented. Model resolution determines how accurately the scale dependence of physical processes is captured and imposes limitations on how well emissions and surface heterogeneities can be resolved for realistic simulations of climate processes such as monsoon and extreme events. To address this critical issue, this project will conduct a series of climate simulations using the Community Earth System Model (CESM1) in various configurations focusing on two specific but related aspects of the problem: (1) what is the sensitivity of climate change projections including some water cycles issues to aerosol processes and emission sources, and (2) what is the role of multi-scale water cycle processes in climate change. Addressing these questions will contribute to our overarching goal of characterizing uncertainties in climate change projections.
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Title: Atomistic Simulations of Nanoscale Oxides and Oxide Interfaces

Principal Investigator: Subramanian Sankaranarayanan, *Argonne National Laboratory (ANL)*

Co-Investigator: Ganesh Kamath (*U. Missouri- Colombia*), Sanket Deshmukh (*ANL*), Ram Subbaraman (*ANL*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 120,000,000 processor hours

Research Summary:
Oxides are chemical compounds that contain oxygen and are important to many sciences and applications. Everyday examples include aluminum oxide on aluminum foils and iron oxide (rust). Nanoscale oxides (oxide materials and substances on the order of 10^{-9} meters) have emerged to be of great interest in a wide range of problems including applications ranging from energy conversion to catalysis. The synthesis of oxides is important for controlling the functionality of the oxide material and one of the approaches to tune oxides at room temperature involves the use of an electric field to stimulate oxide growth. This project supports computational research utilizing atomistic simulations such as classical molecular dynamics (MD) with ReaxFF force field to demonstrate the potential of electrical field application for ceramics processing. This integrated simulation-experimental protocol will determine the way that electrical field application affects the transport processes during oxidation, oxide growth, sintering and how these can be exploited in practical processes and applications. The knowledge acquired can impact the ceramics' processing field, in particular, the design of oxide ceramics and their interfaces that have enhanced microstructural, mechanical and electrical properties compared to their counterparts processed through alternative methods will allow effective integration of electrical field applying techniques into novel processing routes tailored towards customized fabrication of materials.

Title: Dynamics of Conformational Transition in Polymer Grafted Nanoparticles

Principal Investigator: Subramanian Sankaranarayanan, *Argonne National Laboratory (ANL)*

Co-Investigator: Ganesh Kamath (*U. Missouri- Colombia*), Sanket Deshmukh (*ANL*), Derrick Mancini (*ANL*)

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 170,000,000 processor hours

Research Summary:
Polymers are organic molecules and materials synthesized by linking together identical building blocks and are important across many utilization areas including life-sciences, every day materials, and nanotechnology. The possibility of being able to engineer stimuli-sensitive polymers onto surfaces offers incredible potential in medical (wound dressing), bio-medical (medical devices, drug release, anti-bacterial coatings) and micro-engineering (micro-fluidics) applications. Building and engineering these polymer devises, however, is a complex task. Polymer grafted nanoparticles is an approach for controlling the design and functionality of polymers where the polymers are grafted (attached) onto nanoparticles. Properties of the synthesized polymer grafted nanoparticle depend not only on the polymer itself but also on the grafting density and interplay of chain deformation (stretching), excluded volume effects (properties/quality of solvent), and interactions between polymer and a substrate to which it is attached. As such, conformational dynamics (the natural movement of the polymer) are very important to the function and design of the polymer grafted nanoparticle yet the link between specific molecular (microscopic) and macroscopic properties is still not clearly understood. This project supports the use of computational techniques for understanding conformational dynamics by gaining atomistic level insights into the interactions between polymer-water and polymer-polymer and substrate-polymer. Results from these simulations will be compared with the ongoing experiments being carried out at the APS division at ANL. The outcome of the research will further our understanding of how to design, tune and control the functional properties of polymer coated nanoparticles.

Title: High-Resolution Coupled Climate Simulations on Titan with GPU Acceleration

Principal Investigator: Mark Taylor, *Sandia National Laboratories*

Co-Investigators: Valentine Anantharaj (*ORNL*), Kate Evans (*ORNL*),Matt Norman (*ORNL*), David Bader (*LLNL*), Peter Caldwell (*LLNL*), Phil Jones (*LANL*), Mathew Maltrud (*LANL*), Julie McClean (*Scripps Institution of Oceanography*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 64,000,000 processor hours

Research Summary:
Climate models have been used successfully to investigate the impacts of future climate change. Current models, although useful, cannot be used to project potential impacts at the regional and local scales because of their low spatial resolutions (typically, 100km). In addition, many small-scale processes that are unresolved in current models can have significant impact on the global-scale. High-resolution models are required for more accurate simulations of global change and for exploring regional impacts of that change. However, running any Earth system models at high resolution is particularly challenging because multi-decade climate-length simulations require performing millions of timesteps with complex models represented by close to 1M lines of code. This project will perform very high resolution coupled climate simulations (10-25km) to evaluate how small-scale processes influence large-scale climate and how such simulations can inform regional climate impacts, especially extreme events. The project goal is to test the hypothesis that higher resolution models 1) can be made accurate a t the local level and include low-probability events that have feedbacks on large scale climate features and 2) are needed to account for small scale events that have feedbacks on large scale climate features. The outcomes of this project will be a greater understanding of climate modeling and advances in predicting climate impacts on the regional scale.

Title: V/UQ Assessment of a Large Eddy Simulation Tool for Clean-Coal Technology

Principal Investigator: Jeremy Thornock, *U. of Utah*

Co-Investigators: Todd Harman (*U. Utah*), John Schmidt (*U. Utah*),Martin Berzins (*U. Utah*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 7,000,000 processor hours

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Research Summary:

Rising concerns over climate change and an increasing demand for energy both nationally and globally requires that the United States and the world explore clean, cheap sources of energy. Currently, US coal fired power plants are producing nearly 48% of the nation's energy supply, making clean coal technologies highly desirable. This project will use simulation science to explore ways to improve clean coal technologies for the generation of electric power. Using a combination of simulations and industrial experimental data, this project will investigate coal combustion under oxy-coal conditions. The study will include flame stability, variability of inlet conditions, including recycle rates and coal types and coal ignition within the boiler. The end result of these simulations is to demonstrate the predictive capabilities of large scale Large Eddy Simulations (LES) in the design and development of industrially sized boilers. This goal will enable investigation of performance enhancements to (1) minimize the time to solution and (2) deliver quantifiable and predictable technologies that will improve the design of industrially sized coal fired boilers. With these new boiler designs the environmental impact will be lessened by the reduction in GHG emissions while still relying on the United States most abundant natural resource.

Title: Chombo-Crunch: Advanced Simulation of Subsurface Flow and Reactive Transport Processes Associated with Carbon Sequestration

Principal Investigator: David Trebotich, *Lawrence Berkeley National Laboratory (LBNL)*

Co-Investigators: Brian Van Straalen (*LBNL*), Terry Ligocki (*LBN*L), Carl Steefel (*LBNL*), Sergi Molins (*LBNL*)

ALCC allocation: Processor Hours

Site: Argonne National Laboratory
Allocation: 80,000,000 processor hours

Site: Lawrence Berkeley National Laboratory
Allocation: 20,000,000 processor hours

Research Summary:
Carbon sequestration, the process of capturing carbon dioxide (CO2) before it enters the atmosphere and transferring it into the earth, is a promising technology to help reduce greenhouse gases and attenuate climate change. Key to the realization of geologic sequestration of CO2 are new investigative tools for understanding molecular-to-pore-scale processes in fluid-rock systems in order to control critical aspects of flow and transport in porous rock media. One important investigative tool is simulation of reactive transport processes in realistic pore space obtained from image data of CO2 injection experiments. We have developed multiscale, multiphysics simulation tools in the Chombo software framework for high performance simulation capability of flow and transport in complex micro-scale geometries obtained from image data. This technology has been successfully combined with the complex geochemistry module of CrunchFlow to deliver high performance flow and reactive transport modeling in synthetic and realistic packed bed systems. The new capability, called Chombo-Crunch, will enable simulations of the image data problem at realistic time scales and at better than image data grid resolution. The successful completion of these simulations will validate and inform the experiments *a priori* and aid experimental interpretation for future developments in geologic carbon sequestration.

Title: Petascale Simulation of Laser Plasma Interactions Relevant to Inertial Fusion Energy

Principal Investigator: F.S Tsung, *UCLA*

ALCC allocation: Processor Hours
Site: Argonne National Laboratory
Allocation: 40,000,000 processor hours

Research Summary:

Fusion energy is a highly desirable source for clean energy, potentially producing large amounts of energy from a nearly unlimited supply of fuel without long-lived radioactive waste products. Inertial fusion energy (IFE) is one of the most attractive approaches to harness fusion energy. However, ignition, where the fuel burns in a self-sustained way, must be demonstrated first in the laboratory. In late 2012, the ignition campaign at the National Ignition Facility (NIF) ended without ignition in part due to excessive stimulated Raman scattering (SRS) from the laser plasma interactions. An understanding of laser plasma interactions is therefore essential for the success of IFE. Recent advances in hardware and code developments have enabled, for the first time, kinetic simulations of IFE-relevant laser plasma interactions in multiple dimensions. This project will address this critical challenge by supporting developments in IFE experiments through HPC simulations of laser plasma interactions relevant to IFE. The outcomes will significantly advance the understanding of laser plasma interactions relevant to inertial fusion energy.

Title: Transforming Modeling & Simulation for Nuclear Energy Applications

Principal Investigator: John A. Turner, *Oak Ridge National Laboratory (ORNL)*

Co-Investigators: Mark Christon (*LANL*), Thomas E. Evans (*ORNL*), Derek Gaston (*INL*), Douglas B. Kothe (*ORNL*), Roger Pawlowski (*SNL*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 20,000,000 processor hours

Research Summary:
Important challenges for the performance of nuclear reactors include safety, capital costs, and nuclear waste reduction. Due to the prohibitively high costs associated with experimental research, modeling and simulation (M&S) of nuclear reactors is critical for addressing these challenges. The Consortium for Advanced Simulation of Light Water Reactors (CASL) is a U.S. Department of Energy (DOE) Energy Innovation Hub established for M&S of nuclear reactors. CASL applies existing M&S capabilities and develops advanced capabilities to create a usable environment for predictive simulation of light water reactors (LWRs). This environment, the Virtual Environment for Reactor Applications (VERA), incorporates science-based models, state-of-the-art numerical methods, modern computational science and engineering practices, and uncertainty quantification (UQ) and validation against data from operating pressurized water reactors (PWRs), single-effect experiments, and integral tests. This proposal supports the development and application of models, methods, data, and understanding to address three areas of nuclear power plant (NPPs) performance: reducing capital and operating costs by enabling power upgrades and lifetime extension for existing NPPs and by increasing the rated powers and lifetimes of new NPPs; reducing nuclear waste volume generated by enabling higher fuel burnup, and enhancing nuclear safety by enabling high-fidelity predictive capability for component performance through the onset of failure. The outcome of this project will be increased prediction capabilities for the performance of nuclear reactors through comprehensive, science-based modeling and simulation technology that is deployed and applied broadly throughout the nuclear energy industry to enhance safety, reliability, and economics**.**

Title: Investigation of Plasma Rotation Inversion and Profile Structure in Magnetic Fusion Experiments

Principal Investigator: Weixing Wang, *Princeton Plasma Physics Laboratory (PPPL)*

Co-Investigators: Stephane Ethier (*PPPL*), Edward Startev (*PPPL*),Jin Chen (*PPPL*), Zhixin LU (*UCSD*), Patrick Diamond (*UCSD*), George Tynan (*UCSD*),

ALCC allocation: Processor Hours

Site: Lawrence Berkeley National Laboratory

Allocation: 5,000,000 processor hours

Research Summary:

Fusion energy holds promise for being a clean and renewable source of energy for humanity worldwide. Magnetic confinement fusion reactors (e.g. the International Thermonuclear Experimental Reactor) hold great promise as a mechanism for harnessing fusion energy. It is generally believed that the prospects for achieving high quality plasma performance in magnetic fusion devices will be significantly enhanced by optimizing plasma flow characteristics in fusion devices, which plays a critical role in both controlling macroscopic and microscopic processes in fusion plasmas. This project will use gyrokinetic simulations, jointly with theoretical and experimental studies, to investigate plasma flow profile structure under various experimental conditions. The goal of this project is to develop the needed understanding for realistically simulating and modeling plasma flow formation process, and ultimately, strong knowledge base for flow optimization in magnetic fusion devices.

Title: Understanding Helium Plasma Mediated Tungsten Surface Response that Controls Plasma Facing Component Performance and LIfetime

Principal Investigator: Brian Wirth, *Oak Ridge National Laboratory (ORNL)*

Co-Investigators: David Bernholdt (*ORNL*)

ALCC allocation: Processor Hours

Site: Argonne National Laboratory
Allocation: 7,500,000 processor hours

Site: Oak Ridge National Laboratory
Allocation: 5,000,000 processor hours

Research Summary:
The realization of fusion as a practical, 21st Century energy source requires improved knowledge of Helium plasma (He plasma) interactions with material surfaces. The improved knowledge can be used in the materials engineering and design efforts of component systems to survive the incredibly extreme heat and particle flux exposure conditions of a fusion power plant. An important component for the International Thermonuclear Experimental Reactor (ITER) device (an under-construction fusion reactor) is the divertor, which extracts unwanted heat and ash from the plasma during the fusion process. The objective of this project is to further advance understanding of the response of tungsten, the proposed material for the ITER divertor, to low energy He plasma exposure. Knowledge of He interaction with tungsten is necessary to identify materials design strategies to effectively manage high gas exposures expected in the fusion energy environment. This project will perform simulations at both the atomistic and continuum scale for comparison and benchmarking, as well as the identification of appropriate reduced-parameter models to describe complex, multiscale phenomena controlling gas behavior in fusion materials. The outcome will be a greater physical understanding and predictive modeling capability for materials design of the divertor for ITER.

Title: Accelerated Modeling of Non-icing Surfaces for Cold Climate Wind Turbines

Principal Investigator: Masako Yamada, *GE Global Research*

Co-Investigators: Azar Alizadeh (*GE Global Research Center*)

ALCC allocation: Processor Hours
Site: Oak Ridge National Laboratory
Allocation: 40,000,000 processor hours

Research Summary:

Prevention of ice accretion on surfaces is pertinent in many fields, including energy, transportation and telecommunications. In addition to improving operation safety and reducing cost, reduction of ice buildup can lead to increased energy efficiency. For instance, ice buildup on wind turbine blades in cold climates drastically reduces the efficiency of power generation, often requiring turbine shutdown. Many of the current approaches to address ice accumulation are based on *active* processes requiring significant energy to generate heat. Therefore, development of *passive* ice mitigation strategies that require no additional energy is highly desirable. A challenge for passive ice mitigation is that the relationship between hydrophobicity (how resistant a substance is to liquid water 'sticking' to it) and icephobicity (how resistant a substance is to ice 'sticking' to it) is a topic of lively debate. For example, a hydrophobic surface at room temperature may not be icephobic at freezing temperatures, whereas a hydrophilic surface at room temperature may prove icephobic. This project will use simulation modeling to gain insight into the underlying statistics governing freezing and to confirm the efficacy of simulation codes. Outcomes of this work will be to understand the underlying statistics governing nucleation (earliest stages of ice formation) and rapidly screen candidate surfaces for improved resistance to ice accretion in future technologies and infrastructure.